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Nuclear Theory for Nucleosynthesis

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Nuclear structure and reaction theories play crucial roles for advancing our knowledge of nucleosynthesis in astrophysical environments. The status of relevant theoretical formalisms and tools is briefly summarized and areas in need of development are highlighted.

Exploring nucleosynthesis scenarios necessitates simulating both the astrophysical sites considered and the possible nucleosynthesis mechanisms. The most important nuclear properties required in this context are nuclear masses and nuclear reaction rates, primarily for the capture of neutrons, protons, alpha particles on a variety of targets, and cross sections for transfer reactions and nuclear fission. Existing nuclear structure descriptions and nuclear reaction theories will have to be refined and extended to meet the needs of nuclear astrophysics. In some instances, new theories will have to be developed to address the challenges posed by isotopes away from stability, both neutron-rich and neutron-poor species.

Nuclear structure theories range from microscopic *ab initio* approaches to macroscopic phenomenological descriptions. A variety of approaches is required in order to connect to experimental observations, to identify systematic trends, to guide and test theories across the nuclear chart. The various shell models (*ab initio* No-Core Shell Model, Traditional Shell Model, Monte-Carlo Shell Model, Shell-Model Monte Carlo approach, Symmetry-Adapted Shell Model, Continuum Shell Model, etc.), the Green-Function Monte-Carlo approach, Coupled-Cluster Model, Density-Functional Theories (DFT) and 'Beyond-Mean-Field' Theories (RPA, QRPA, continuum RPA) find application in different, but overlapping areas of the nuclear chart and need to be enhanced and extended in order to connect to each other, to cover the isotopes of interest, and to provide the structure input required by nuclear reaction theories. Similarly, nuclear reaction theories (Faddeev, Faddeev-Yakubovsky, Alt-Grassberger-Sandhas formulations, R-matrix theory, single-channel and coupled-channels direct reaction theories, multi-step direct and multi-step compound descriptions, statistical Hauser-Feshbach theory, etc.) need to be revised and extended in order to make use of newly-available (experimental and theoretical) structure information and vastly-improved computational capabilities if they are to address the wide range of nuclear physics issues relevant to astrophysics. In addition, structure and reaction theories need to be more closely integrated with each other.

Nuclear theory challenges that are particularly relevant to astrophysics include the need to extend current descriptions i) from laboratory to stellar energies, and ii) from stable nuclei to exotic, short-lived isotopes. Expanding the reach of theory to

these novel regimes requires a comprehensive understanding of the reaction mechanisms involved (including direct, semi-direct, pre-equilibrium, compound processes), as well as detailed knowledge of the nuclear structure (including particle thresholds, single-particle and cluster structure, collective phenomena) and mechanisms for incorporating feedback from experiment. Many nuclei of interest have to be treated as open many-body systems and special consideration of stellar environments need to be included (role of excited states, electron screening mechanisms).

Nuclear structure theory is needed to predict properties of isotopes that play a role in astrophysical environments. Ground states as well as excited states of stable and exotic nuclei are of interest. Ideally, continuum effects are included in the description.

Ab initio approaches (which describe the nucleus using a well-defined microscopic Hamiltonian with A nucleon degrees of freedom, treat the internal relative motion correctly, and obtain the relevant observables by solving the quantum many-body equations without uncontrolled approximations) have made considerable progress over the past decade in describing light nuclei. Growing computational resources and improved numerical algorithms, a move from realistic phenomenological and meson-theoretical nucleon-nucleon potential models to nuclear interactions derived from chiral perturbation theory, the inclusion of three-nucleon (and even more-nucleon) forces, and the inclusion of the continuum are showing their effects in nuclear astrophysics. *Ab initio* approaches can now treat reactions such as $^3\text{H}(d,n)^4\text{He}$, $^3\text{He}(d,p)^4\text{He}$, $^7\text{Be}(p,g)^8\text{B}$, etc. An accurate description of the ^{12}C Hoyle state, which has been identified as a major problem in nuclear astrophysics, is a near-term goal, and we can expect that modern methods will solve another longstanding problem, namely a theoretical description of the $^{16}\text{O}(\alpha,\gamma)$ reaction.

While extensions of the *ab initio* approaches push towards the treatment of systems with $A > 16$, predictions of nuclear energies, spectroscopic factors, level densities, electromagnetic multipole transitions, Gamow-Teller strength functions, and other properties of medium-mass nuclei are typically made using the large-basis traditional shell model, the shell-model Monte-Carlo approach, or Density-Functional approaches and their extensions. Here research is focused on improving effective Hamiltonians and pushing the computational boundaries. Complementary developments are underway to extend the reach of *ab initio* approaches by using symmetry-adapted bases to overcome model-space limitations. These developments are important for obtaining improved predictions for γ and β strength functions, which are needed for nucleon capture calculations and predicting β -decay rates, respectively.

Nuclear properties of heavier systems ($A > 100$) are typically obtained from density-functional theories and approaches that include correlations beyond DFT, such as the Random-Phase Approximation (RPA) and the Quasi-Particle RPA. Recent work

in the context of DFT has focused on improving the energy-density functional itself and on quantifying uncertainties; a long-term effort to derive a functional from the underlying forces has been initiated. Such efforts are important for obtaining mass predictions with associated uncertainties. Correlations beyond those included in DFT approaches are critical for calculating strength functions, such as those needed as input for statistical reaction calculations and for predicting β -decay rates. (Q)RPA calculations are technically challenging, but have benefited from increasing computational capabilities and new numerical techniques, making it possible to remove some of the approximations used in the past. For instance QRPA calculations for deformed nuclei, using a finite-range interaction, are now possible. Work remaining to be done includes: further computational improvements, to make a wider range of calculations feasible, and the inclusion of couplings to more complicated excitations and the continuum to properly predict spreading of unbound states and decays. Such developments will be valuable for reliably calculating properties of excited states and for providing microscopic input for reaction calculations.

As the r-process reaches nuclei in the mass region of $A=200-250$, fission will occur, which can significantly impact the nucleosynthesis yields through fission recycling. Current astrophysics models use phenomenological fission models that rely on model parameters that are typically fit to existing data. These models have insufficient predictive capability. Improvements are expected to come from microscopic fission theories that make use of Density Functional Theory. Progress has been made in this area in recent years, even fission in a plasma environment is being considered, but both formal and computational challenges remain to be overcome to properly describe the complex processes involved.

Two goals of **nuclear reaction theory** are particularly relevant to astrophysics: 1) Achieving a comprehensive description of direct, semi-direct, pre-equilibrium, and compound processes for a variety of reactions, and 2) Extracting astrophysically-relevant quantities from combinations of theory and indirect experiments.

Reaction theory is needed to describe elastic and inelastic scattering processes, the fusion of nuclei, as well as transfers of nucleons or groups of nucleons between projectile and target. The complexity of the problem requires the elimination of possible reaction channels from explicit consideration and the introduction of optical potentials. Phenomenological optical potentials have received much attention in the past decade. The availability of a wide range of experimental data, coupled with current computational capabilities, has led to greatly improved parameterizations, in particular for nucleon-nucleus reactions. The development of optical potentials for reactions that involve deuterons or other light ions is making much-needed progress. Further improvements are needed to achieve better accuracy and to describe reactions with isotopes away from stability. This will involve including deformation and non-locality effects in the potentials and possibly revising codes that use these potentials as input. In order to reliably treat regions away from stability microscopic optical-model approaches will be needed.

Low-energy binary reactions proceeding through isolated resonances are described by R-matrix theory. Typically, measured cross sections are fit by adjusting phenomenological R-matrix parameters, a procedure which allows the extraction of resonance properties and extrapolation to energy regimes for which no data is available. State-of-the-art codes have implemented multi-level and multi-channel treatments. Improvements should include the use of (calculated) structure data and extensions to treat transfer reactions that involve resonances.

Reactions involving the capture of neutrons, protons and other charged light ions, play an important role in astrophysics. Cross section calculations require reliable optical potentials. To improve the calculations of direct-capture processes, deformation should be treated consistently and the contributions from semi-direct capture need to be considered. Capture proceeding via the formation of a compound nucleus is described in a statistical model, typically a Hauser-Feshbach approach.

Multiple Hauser-Feshbach codes for the description of compound-nuclear reactions (including capture) are publicly available, well documented, supported, and user-friendly. These codes require nuclear structure input (discrete levels, level densities, gamma-ray strength functions, fission barriers, etc.) and optical models, as well as pre-equilibrium descriptions. Current codes make use of available nuclear structure databases and include a range of phenomenological models to provide the required inputs. Moreover, the past decade has seen a move towards the use of microscopic approaches for calculating the needed inputs. Continuing these efforts is important for achieving more reliable predictions for unstable nuclei. Additional, potentially significant, improvements include an explicit treatment of deformation effects, more emphasis on fully quantum-mechanical descriptions of pre-equilibrium processes, and a better understanding of correlations between different reaction channels (width fluctuation corrections).

More generally, the interplay between direct reactions, semi-direct processes, pre-equilibrium contributions, and compound reactions is not sufficiently understood. The influence of doorway states (simple configurations that couple the reaction entrance channel to more complex configurations) needs to be considered and the issue of energy averaging needs to be revisited. A better understanding of these issues will yield more reliable cross section calculations. This is particularly significant describing low level-density regions away from stability, but it also impacts stable nuclei, e.g. in the Fe region and near closed shells.

Additional areas in need of attention are charge-exchange reactions (which have not received much attention recently), electron screening effects and reactions on excited states (which can be expected to play a role in astrophysical plasma environments), and nuclear reactions in the presence of strong magnetic fields. An effort needs to be made to include theoretical uncertainties with the reaction calculations, as errors need to be propagated in the astrophysical models that use the reaction theory results.

Indirect measurements will play an increasingly important role in nuclear astrophysics as the focus moves towards improving our descriptions of unstable isotopes for which properties and reaction cross sections cannot be measured directly or calculated reliably. The observables obtained from such measurements have to be related to the quantities desired, which requires reaction theory. The most important quantities one would like to extract from measurements are resonance properties (resonance energies and widths), cross sections for direct capture of charged particles, and compound-nuclear cross sections. The most likely indirect approaches used will employ radioactive-beam experiments involving inelastic scattering and transfer reactions, such as (d,p) reactions.

Current reaction theories have to be extended to reliably link the measurements to the desired information. For deuteron-induced reactions, it is important to treat both the transfer and the breakup contributions. Recent work has shown that it is important to improve the treatment of the three-body dynamics in (d,p) reactions. A reliable description of transfers to (both wide and narrow) resonance states, which would allow the extraction of resonance parameters, does not exist. Further, the interplay of direct and compound processes is not sufficiently understood for both inelastic scattering and transfer reactions. These shortcomings will affect the interpretation of radioactive-beam experiments that aim at extracting nuclear structure information as well as indirect measurement that aim at determining compound cross sections.
